Methyl parathion 298-00-0 | DTXSID1020855

Model	Data

Weighted KNN model

5-fold CV	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 6.64e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.49e-01

Confidence level: 6.48e-01

Nearest Neighbors from the Training Set

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Thionazin

Measured: 3.50e-06 Predicted: 8.23e-05

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Cyclonite

Measured: 5.40e-05 Predicted: 8.96e-09

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Chlorfenvinphos

Measured: 4.00e-06 Predicted: 3.27e-06

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4,5-Dichloroguaiacol

Measured: 3.60e-06 Predicted: 2.47e-03

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Parathion

Measured: 6.68e-06 Predicted: 7.67e-06